

High Performance Multi Barrier Thermionic Devices

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ABSTRACT

Thermoelectric transport perpendicular to layers in multiple barrier superlattice structures is investigated theoretically in two limiting cases of no lateral momentum scattering and strong scattering. In the latter regime when lateral momentum is not conserved, the number of electrons participating in thermionic emission will dramatically increase. The cooling power density is calculated using Fermi-Dirac statistics, density-of-states for a finite quantum well and the quantum mechanical transmission coefficient in the superlattice. Calculation results show that metallic based superlattices with tall barriers (>10 eV) can achieve a large power factor on the order of 0.06W/mK^2 with a moderate electronic contribution to thermal conductivity of 1.8W/mK . If the lattice contribution to thermal conductivity is on the order of 1W/mK , ZT values higher than 5 can be achieved at room temperature.¹

INTRODUCTION

Thermoelectric *figure-of-merit*, ZT specifies how “good” the material is for thermoelectric cooling and power generation applications. Widely used thermoelectric material at room temperature is based on Bi_2Te_3 .² Heterostructure Integrated Thermionic (HIT) coolers have been recently made and characterized for applications in integrated cooling of optoelectronic and electronic devices^{3,4,5,6}. The idea of thermionic energy conversion was first seriously explored in the mid fifties during the development of vacuum diodes and triodes. Vacuum diode thermionic refrigerators were proposed by Mahan in 1994.⁷ Efficiencies over 80% of the Carnot value were predicted, but the operating temperatures are still limited to greater than 500K .

MULTI BARRIER THERMIONIC DEVICES

Thermionic emission cooling in heterostructures was proposed by Shakouri *et al.*³ to overcome the limitations of vacuum thermionics at lower temperatures. In these structures, a potential barrier is used for selective emission of hot electrons and evaporative cooling of the electron gas. The HIT cooler can be based on a single barrier or a multi barrier structure. In a single barrier structure in strong nonlinear transport regime, electron transport is dominated by the supply of electrons in the cathode layer and large cooling power densities can be

achieved.³ However, energy conversion efficiency in these structures is very low. On the other hand, in a multi barrier structure in linear transport regime, one can define an effective Seebeck coefficient and electrical conductivity. In linear transport regime calculations based on an effective conventional thermoelectrics or solid-state thermionics will converge and they represent two points-of-views for the same electron transport phenomena in superlattices. One can describe the effect of potential barriers as a mean to increase the thermoelectric power factor (Seebeck coefficient square times electrical conductivity). Calculations presented in references [1,8] show that the conservation of lateral momentum for electron transport perpendicular to superlattice layers plays an important role in achieving high ZT values. In the following, we will study the thermionic energy conversion efficiency in superlattices in quasi linear transport regime. We will specifically examine the two cases of conserved and non-conserved lateral momentum. As a concrete example, thermoelectric properties of InGaAs/InAlAs superlattices is studied. Material properties of these superlattices are very well characterized for applications in intersubband quantum well infrared photodetectors and quantum cascade lasers. Structure and material parameters are tabulated in table 1:

n_w	L_w (nm)	L_b (nm)	E_b (meV)	m_{eff} (well/barr)	β (W/mK)	v_s (cm/s)	α (eV^{-1})
50	20	10	520	0.043/0.069	5	2×10^7	1.167

where n_w is number of superlattice periods, L_w (L_b) is the well (barrier) thickness, E_b is barrier height, β is thermal conductivity of the whole structure, v_s is electron saturation velocity and α is the non-parabolicity coefficient of the energy band. Mobility values in the well and barrier regions depend on doping concentrations and are determined using the following empirical quantities:

$\mu_w (\text{cm}^2 / \text{Vs}) \cong 37666 - 1845.61 \times \log N_D (\text{cm}^{-3})$ in the well, InGaAs, region and

$\mu_b (\text{cm}^2 / \text{Vs}) \cong 5614 - 276.38 \times \log N_D (\text{cm}^{-3})$ in the barrier, InAlAs, region.⁹

N_D is the doping concentration in each region. An average mobility value has been used for the calculation of the cooling power densities. It is also assumed that both well

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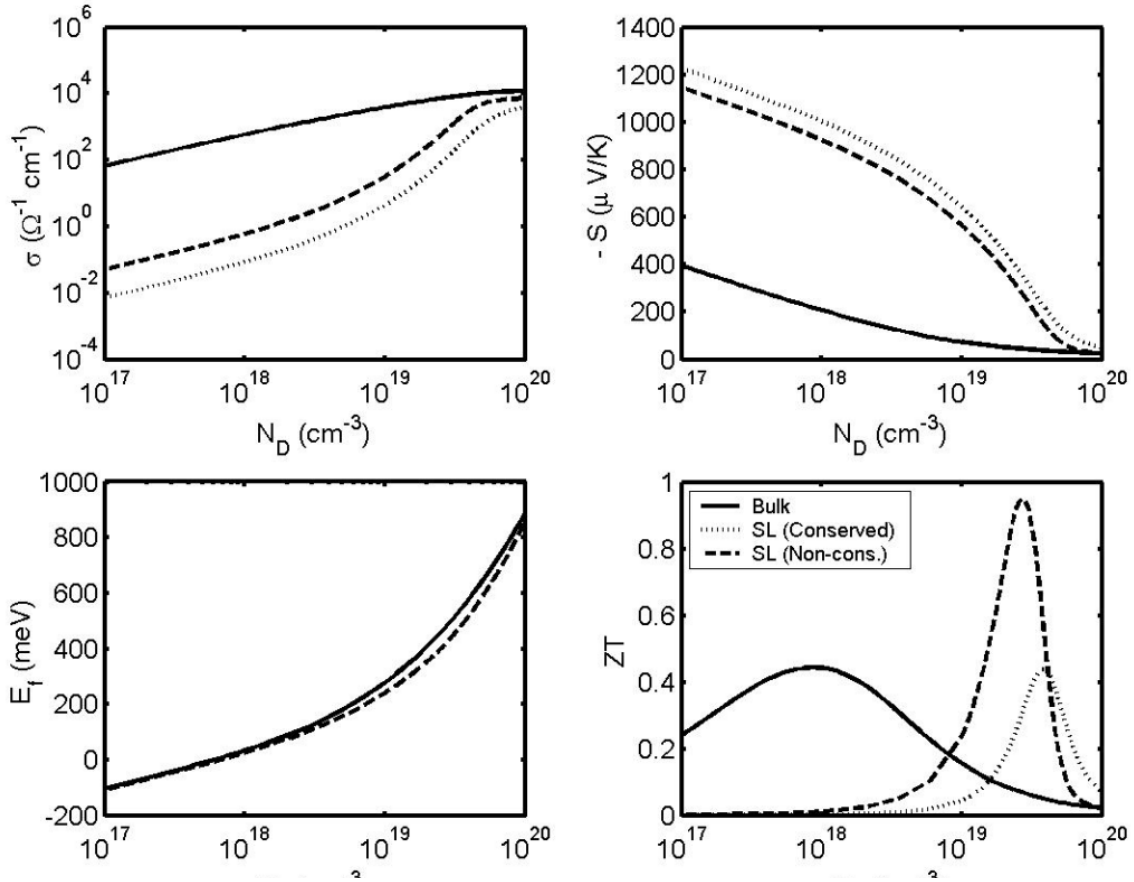


Figure 1: Electrical conductivity (left-top), Fermi energy (left-bottom), Seebeck coefficient (right-top), and Thermoelectric Figure-of-Merit (right-bottom) of InGaAs/InAlAs superlattice for three cases of bulk (solid), superlattice conserved (dotted), and superlattice non-conserved (dashed) lateral momentum cases at $T=600\text{K}$. A bulk lattice thermal conductivity of 5W/mK is assumed for all three structures.

and barrier regions are uniformly doped. Figure 1 shows the calculated electrical conductivity, σ , effective Seebeck coefficient, S , Fermi energy, E_f , and the effective thermoelectric figure-of-merit, ZT , for InGaAs bulk and InGaAs/InAlAs superlattice at the temperature of 600K . For the superlattice, two cases when the lateral momentum is and is not conserved are considered.

This result is similar to previous studied on thermionic/thermoelectric refrigeration¹⁰. However, there are several assumptions made in order to reach this result. Thermionic current has contributions from both two-dimensional (2D) states in the well and three-dimensional (3D) states with energies above the barrier. Superlattice structure chosen here has wide wells with several quantized states that reduce the effect of 3D states on thermionic current. A more important assumption is that the lateral momentum of electrons is assumed to be conserved. As we see in the plot, violation of this assumption can make a significant difference in

Conductivity of superlattice is reduced due to the selective emission of electrons over the barrier. Although the Seebeck coefficient is increased in superlattice structure, the optimum figure-of-merit is about the same as the bulk InGaAs when the lateral momentum is conserved. This is due to the significant conductivity reduction in superlattice structure.

conductivity and ZT . In this case thermoelectric figure-of-merit ($ZT \sim 0.95$) is about two times larger than that in bulk material ($ZT \sim 0.44$). Models similar to that in [10] do not converge to bulk when the barrier height (E_b) is reduced to zero. However, our model has this advantage that when E_b goes to zero, ZT of superlattice converges to that of bulk. It can be seen that at low doping, when the Fermi energy lies deep in the well, conductivity of superlattice is several orders of magnitude less than that of bulk. However, as the doping increases, three dimensional (3D) states above the barrier participate more in thermionic current and conductivity increases

accordingly. When the Fermi energy reaches near the barrier edge, conductivity of superlattice is almost equal to that of bulk. It is important to note that thermal conductivity is often reduced in superlattice structures. To emphasize the cooling improvement solely due to the thermionic emission of electrons over the barrier, the reduced thermal conductivity is not included in the above analysis.

THERMIONIC ENERGY CONVERSION IN METALLIC SUPERLATTICES

A maximum ZT of an InGaAs alloy happens at doping concentrations of 3.5×10^{17} which corresponds to Fermi energy equal to 28.6 meV above the conduction band edge. In this case, while the Seebeck coefficient is relatively high, electrical conductivity is low resulting in a low ZT of about 0.05 at room temperature. Conversely, metals have a large number of free electrons, which contribute to electrical conductivity, and they would be ideal candidate for thermoelectric energy transport. However, metals have very low Seebeck coefficients which results in low thermoelectric figures of merit (ZT). The low Seebeck coefficient is due to the fact that when the Fermi energy is deep inside the conduction band, the contribution of electrons with different energies to the conduction process (differential conductivity) is symmetric with respect to the Fermi energy. An

introduction of tall barriers inside metal will allow the filtering of hot electrons and thus the Seebeck coefficient can be significantly increased. Figure 2 shows the calculated thermoelectric power factor ($S^2\sigma$) versus Fermi energy (E_f). Electronic contribution to thermal conductivity (β_e) for maximum power factor is also shown in the right axis. The results both for conserved and non-conserved cases are shown. A power factor as high as 0.064 W/mK^2 (corresponding to ZT of 6.7, when lattice thermal conductivity is 1 W/mK) is predicted for this structure when the lateral momentum is not conserved. This is due to the higher electrical conductivity and a Seebeck coefficient that resulted from the asymmetric distribution of transported electrons compared to Fermi energy. Optimum barrier height for the maximum power factor is given in reference [1]. Mobility is taken to be $12.2 \text{ cm}^2/\text{Vs}$, value for a typical metal. Thermal conductivity in metals is dominated by electron thermal conductivity that is approximately $2.44 \times 10^{-8} \sigma T$ in units of W/mK according to Wiedemann-Franz law. However, electrical conductivity (σ) in a metallic superlattice is low compared to that in bulk metal, and hence electron thermal conductivity can be comparable to that of phonons in the barrier, as seen in Figure 2.

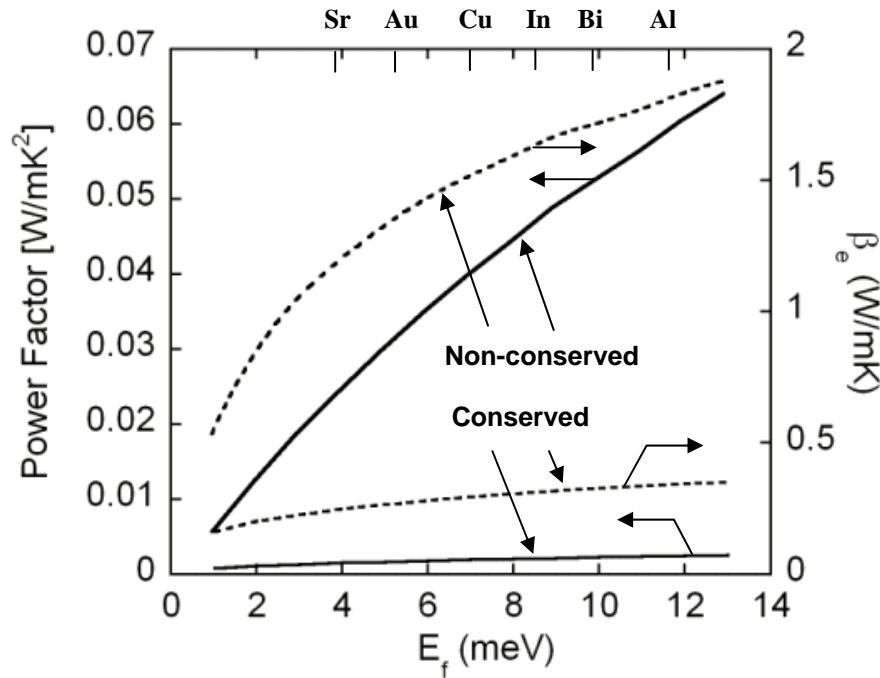


Figure 2: Thermoelectric power factor (left axis) and electronic contribution to thermal conductivity (right axis) vs. Fermi energy for a metallic superlattice.

One should notice that the conservation of lateral momentum plays an important role in determining the number of carriers that participate in the conduction process in metallic superlattices. Its significant influence on power factor is noticeable in Figure 2. Conservation of lateral momentum is a consequence of translational invariance in the plane of quantum well. It is possible by introducing controlled roughness at interface or with embedded quantum dots break this translational invariance and increase the thermionic cooling power density.

CONCLUSION

We have described detailed theory of electron and thermoelectric transport perpendicular to heterostructure superlattices. We studied two limiting cases to determine the number of electrons participating in a thermionic emission process that is based on the conservation of lateral momentum. Non-conserved lateral momentum will dramatically increase the number of electrons that are transmitted over the barrier. These electrons are responsible for thermionic/thermoelectric power conversion, and thereby the effective ZT is increased. Calculations for superlattice structures such as InGaAs/AlGaAs showed that the effective thermoelectric power factor (electrical conductivity times the square of the effective Seebeck coefficient) can be improved comparing to that of bulk material. We also showed that metallic based superlattices with tall barriers can achieve a large effective thermoelectric figure-of-merit ($ZT > 5$ at room temperature) with moderate lattice thermal conductivity of 1W/mK. The improvement in the effective power factor through thermionic emission can be combined with the other methods to reduce the phonon thermal conductivity in superlattices and thus obtain a higher thermoelectric cooling power factor.^{11,12}

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